

# Pre-site Characterization Risk Analysis for Commercial-Scale Carbon Sequestration

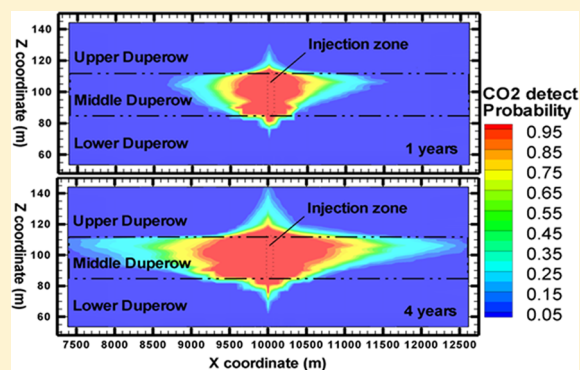
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**ABSTRACT:** This study develops a probability framework to evaluate subsurface risks associated with commercial-scale carbon sequestration in the Kevin Dome, Montana. Limited knowledge of the spatial distribution of physical attributes of the storage reservoir and the confining rocks in the area requires using regional data to estimate project risks during the pre-site characterization analysis. A set of integrated Monte Carlo simulations are used to assess four risk proxies: the CO<sub>2</sub> injectivity, area of review (AoR), migration rate into confining rocks, and a monitoring strategy prior to detailed site characterization. Results show a reasonable likelihood of reaching the project goal of injecting 1 Mt in 4 years with a single injection well (>58%), increasing to >70% if the project is allowed to run for 5 years. The mean radius of the AoR, based on a 0.1 MPa pressure change, is around 4.8 km. No leakage of CO<sub>2</sub> through the confining units is seen in any simulations. The computed CO<sub>2</sub> detection probability suggests that the monitoring wells should be located at less than 1.2 km away from the injection well so that CO<sub>2</sub> is likely to be detected within the time frame of the project. The scientific results of this study will be used to inform the detailed site characterization process and to provide more insight for understanding operational and technical risks before injecting CO<sub>2</sub>.



## INTRODUCTION

CO<sub>2</sub> sequestration in geologic reservoirs is an important approach to mitigating greenhouse gas emissions to the atmosphere.<sup>1–3</sup> The Big Sky Carbon Sequestration Partnership (BSCSP) is one of seven partnerships tasked by the U.S. Department of Energy with demonstrating the feasibility of large scale CO<sub>2</sub> injection into the subsurface. These projects play a significant role in helping to shape our understanding of the interplay between infrastructure, technology, and regulations. The BSCSP is unique among these projects in that CO<sub>2</sub> will be produced from an existing natural accumulation and reinjected down-dip into the same geologic formation.<sup>4</sup> Prior to developing CO<sub>2</sub> injection sites, operators are required to perform a detailed analysis of features, events, and processes (FEPs)<sup>5</sup> that have the potential to impact the environment, human health and safety, economics, and/or project milestones. A FEPs analysis performed for the BSCSP included consideration of the subsurface and resulted in a ranked list based on expert opinion.<sup>6</sup> Subsurface FEPs of concern for the BSCSP project include: risk of insufficient permeability to inject 1 million tonnes CO<sub>2</sub> during the project lifetime; risk of leaked CO<sub>2</sub> impacting overlying drinking water aquifers, which may cause a decrease in groundwater pH and could potentially degrade groundwater quality;<sup>7–22</sup> risk of CO<sub>2</sub> and/or brine escape from the storage reservoirs through overlying confining

rocks via preferential pathways, such as high-permeability zones, faults, and abandoned wells; and risk of ineffective placement of monitoring wells and the resulting inability to detect plume migration.

At the beginning of projects, such as the Big Sky Carbon Sequestration Project, there is often insufficient local geologic data available to perform well-constrained risk analyses of project success. Nonetheless, project operators, funders and regulators require a preinjection risk analysis that identifies potential problem areas and provides guidance on the probability of success. Such analyses can inform early decisions in the site characterization process, such as placement of characterization wells that will later serve as monitoring wells, intervals to core and analyze, appropriate well tests to be performed, and areas to be permitted, that can have an additional impact on probability of success. In the absence of site specific data, this requires that the analysis of subsurface FEPs be performed using numerical simulations that rely on data from the surrounding region. For example, Deng et al.<sup>19</sup> used a field-scale example at the Rock Springs Uplift (RSU),

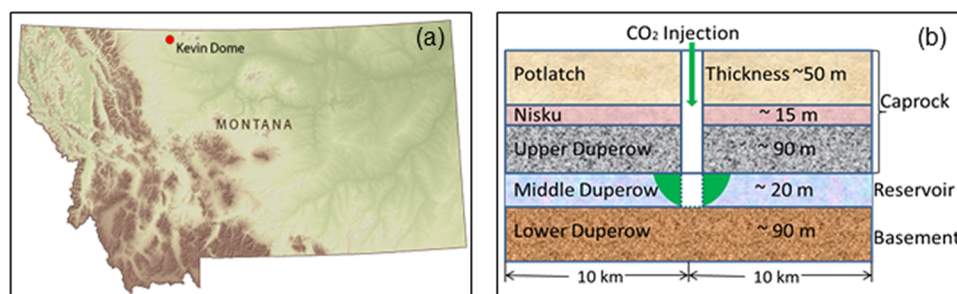
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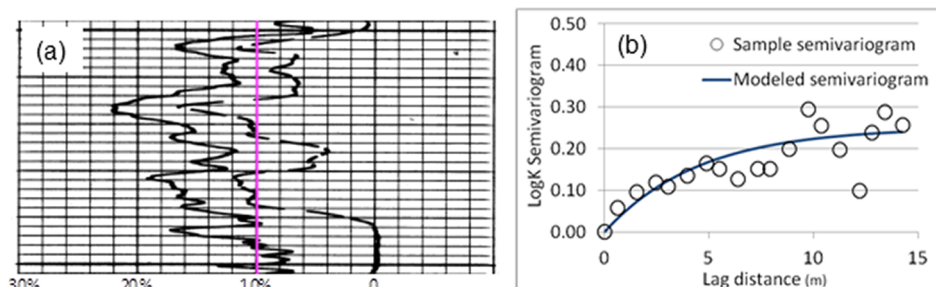
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**Figure 1.** Kevin Dome site location (a) (from BSCSP Web site: [www.bigskyco2.org/research/geologic](http://www.bigskyco2.org/research/geologic)) and a diagrammatic cross section through the injection well (b).



**Figure 2.** Well log data for the middle Duperow with a thickness of 16 m and a porosity bound between 0.05 and 0.22 (a) and the semivariograms of the log permeability (b).

Wyoming, to explore the impacts of reservoir heterogeneity on  $\text{CO}_2$  storage capacity, injectivity, and the potential migration into confining rocks. Their results indicate that reservoir heterogeneity has a large impact on the computed  $\text{CO}_2$  injectivity and the potential migration into confining rocks. Recent drilling at the RSU site has shown that heterogeneity is necessary to correctly represent reservoir injectivity and storage capacity.<sup>23</sup> The present study takes the heterogeneous properties of the reservoir and confining rocks as one of the major factors governing four primary subsurface FEPs and uses the BSCSP's Kevin Dome  $\text{CO}_2$  sequestration site in Montana as an example to demonstrate the usefulness of a probability framework for pre-site characterization risk analysis.

Kevin Dome (see Figure 1a) is a large geologic feature that covers roughly 700 square miles in Toole County, Montana. The Kevin Dome Project (managed by the Big Sky Carbon Sequestration Partnership) will produce 1 Mt (million tonnes) of  $\text{CO}_2$  from a natural source within the dome. The  $\text{CO}_2$  will be transported by pipeline approximately 10 km to the injection site. The target  $\text{CO}_2$  reservoir is at 1100 m depth in the Middle Duperow formation located in the water leg of the Kevin Dome  $\text{CO}_2$  gas deposit. Heterogeneity of the hydrologic properties of the Middle Duperow reservoir and the confining rocks is relatively unknown. Previous studies in nearby oil fields provide some information about the range and distribution of reservoir parameters, such as depth, thickness, permeability, and porosity.<sup>24</sup> We use the statistical distributions of these uncertain parameters to generate Monte Carlo simulations of reservoir performance in order to assist with planning and development of the Kevin Dome sequestration site. The simulations are conducted by coupling the uncertainty quantification tool PSUADE,<sup>25</sup> the Los Alamos developed geostatistical modeling tool GEOST<sup>26,27</sup> modified from the Geostatistical Software Library<sup>28</sup> and the multiphase reservoir simulator FEHM.<sup>29</sup> We use PSUADE to sample distributions of the reservoir and confining rocks and evaluate the statistical distribution of  $\text{CO}_2$

plumes. GEOST is used to generate spatial distributions of heterogeneous parameters for the reservoir and confining rocks from limited borehole log data available outside the site. The reservoir simulator, FEHM, is applied to model the flow of  $\text{CO}_2$  and water in the reservoir and confining rocks for each generated heterogeneous field. Finally, we conduct a preliminary risk analysis using the results of the Monte Carlo simulations to quantitatively evaluate the following risk proxies that relate to the four primary subsurface FEPs: (1)  $\text{CO}_2$  injectivity; (2) radius of the Area of Review (AoR); (3)  $\text{CO}_2$  migration out of the injection horizon; and (4) optimum location of monitoring wells. Risk proxies are defined as measurable quantities that can be used to gain insight into project risk without the need to generate a rigorous consequence structure.

## MATERIALS AND METHODS

**Characterization of Multiscale Heterogeneity.** The Duperow formation within the Kevin Dome site is found at depths ranging from 1000 to 1900 m with a total thickness of between 125 and 260 m. The relatively high-permeability Middle Duperow Formation is the limestone-dolostone injection target reservoir, with thickness between 20 and 58 m (Figure 1b). The permeability values in the Middle Duperow are between 1 and 210 mD with porosity between 0.05 and 0.25. The overlying caprock, consisting of variable dolostone, shale, and anhydrite formations (e.g., Upper Duperow formation, 90 m thick; Nisku formation, 15–23 m thick; and Potlatch formation, about 50 m thick), has a mean thickness around 160 m and a much lower permeability (between 0.001 and 10 mD and porosity 0.01–0.1). Below the target reservoir, the Lower Duperow is used as “basement” in the model. Its thickness is around 90 m and its permeability and porosity distributions are similar to the Upper Duperow Formation.<sup>4,6</sup>

**Statistics of Well Log Data.** There are no site-specific core or log data for the planned injection site. Consequently, we use

Table 1. Parameter Uncertainty for the Kevin Dome Site

uncertain parameters		min.	max.	mean	standard deviation	distribution
reservoir (Middle Duperow)	permeability variance (rVar)	0.1	0.5			uniform
	perm scale (rScale, km)	0.5	5.0			uniform
	anisotropy factor (rFkxz)	1.0	50			uniform
	permeability (rKmean, log m <sup>2</sup> )	−15.6	−11.6	−13.5	0.5	normal
	porosity (rPor)	0.05	0.22	0.08	0.05	normal
confining rocks	porosity (cPor)	0.01	0.12	0.05	0.02	normal
	permeability (cKmean, log m <sup>2</sup> )	−18.6	−14.6	−16.5	0.25	normal
	permeability variance (cVar)	0.1	0.25			uniform

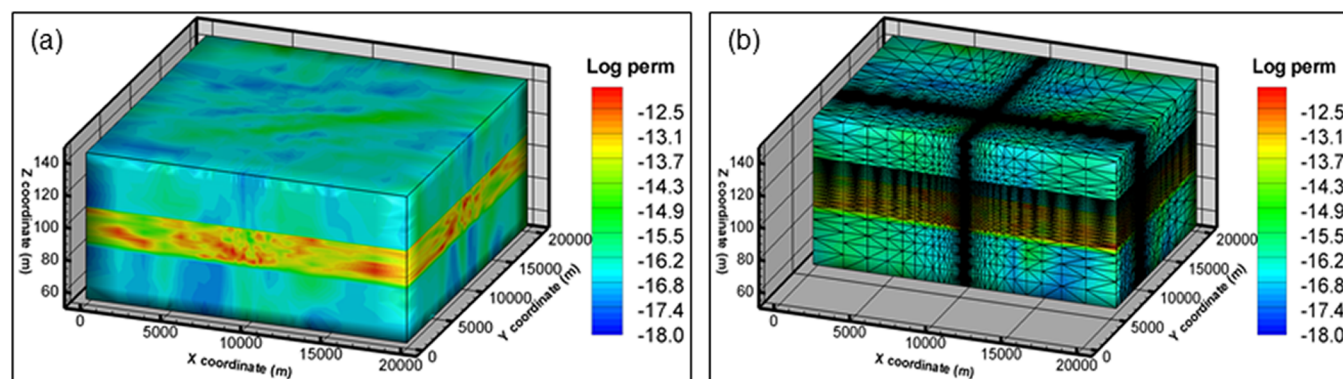


Figure 3. Simulated heterogeneous caprock and reservoir permeability field (a) and numerical grid (b) in 3-D view from one realization.

data from a well, MCFGPD-2175, located within 15 km of the site that penetrates the targeted Middle Duperow injection horizon.<sup>6</sup> The log data from well MCFGPD-2175 were used to define the porosity distributions in the Middle Duperow (Figure 2a). The log curves span a porosity distribution between 0.05 and 0.22. Based on these data we convert the porosity data to permeabilities according to Bernabe et al.<sup>30</sup> and Deng et al.<sup>19</sup>

$$k = a\phi^b \quad (1)$$

where  $k$  is permeability (m<sup>2</sup>),  $\phi$  is porosity,  $a$  and  $b$  are constants as defined in Deng et al.<sup>19</sup>

By using the converted log permeability data we compute the sample semivariograms using eq 2 in the vertical direction and fit the results with an exponential function (eq 3)<sup>28,31</sup>

$$\hat{\gamma}_Y(h) = \frac{1}{2|N(h)|} \sum_{(i,j) \in N(h)} (Y(z_i) - Y(z_j))^2 \quad (2)$$

$$\gamma_Y(h) = \sigma^2(1 - e^{-h/\lambda}) \quad (3)$$

where,  $\hat{\gamma}_Y$  and  $\gamma_Y$  are the sample and modeled semivariograms of log permeability data  $Y$ , respectively,  $N(h)$  is the pair number at a lag distance of  $h$ ,  $z_i$  and  $z_j$  are two points separated by a distance  $h$ ,  $\sigma^2$  is variance, and  $\lambda$  is the integral scale.

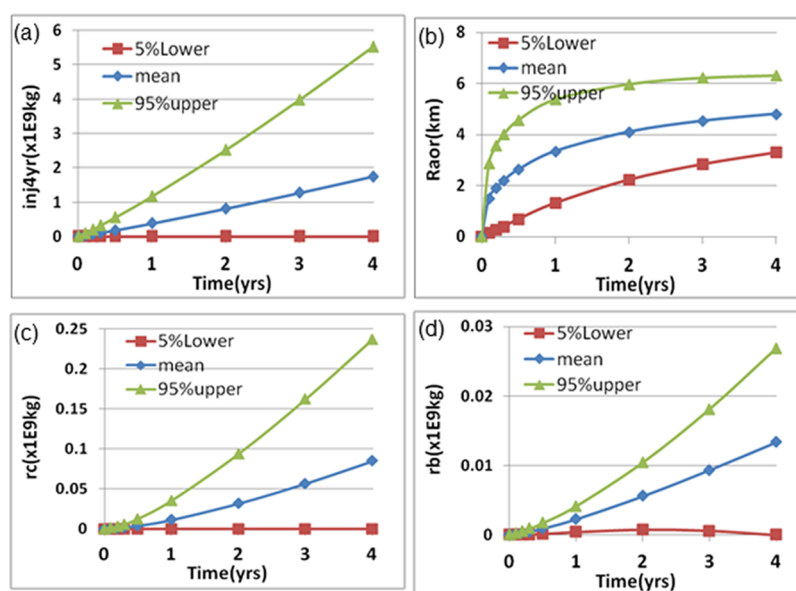
The results for fitting eq 2 with eq 3 are shown in Figure 2b. The estimated statistical parameters of the log permeability are a variance of 0.25, vertical integral scale of 5 m, and mean permeability of  $3 \times 10^{-14}$  m<sup>2</sup>. Based on the variogram analysis results and other regional geological data,<sup>4,24,32</sup> we summarize the ranges and distributions of the uncertain parameters for simulating the heterogeneity of the reservoir and the confining rocks (e.g., caprock and basement) in Table 1. The reservoir and confining rock permeabilities are normally distributed and are positively correlated with the unit porosity. Other

parameters listed in the table satisfy uniform distributions. Having limited existing data, we assume that the lower and upper bounds of the horizontal integral scales are 1000 times larger than those of the vertical integral scales for both the reservoir and the confining rocks. The permeability anisotropy factors for the reservoir and confining rocks are assumed to be the same. The mean permeability in the caprock and basement is 3 orders of magnitude lower than that in the reservoir and the variance is a half of that of the reservoir.

**Parameter Sampling.** PSUADE and GEOST are coupled in our methodology, generating 300 realizations with Latin Hypercube sampling and geostatistical modeling, to perform an integrated Monte Carlo simulation of CO<sub>2</sub> injection and transport in the reservoir, caprock, and basement. For each realization the heterogeneous permeability fields for the reservoir (Middle Duperow), caprock, and basement are simulated with the sequential Gauss method since they have quite different mean permeabilities and variances. An example of a simulated permeability field for caprock, basement, and reservoir is shown in Figure 3.

**CO<sub>2</sub> Injection Simulations.** FEHM is used to simulate CO<sub>2</sub> injection and the subsequent flow of both CO<sub>2</sub> and water at the Kevin Dome injection site for 300 realizations. The computational model size is 20 000 × 20 000 × 280 m with 197 213 nodes. The injection well is located in the center of the model where the grid is highly refined with minimum grid sizes  $dx$ ,  $dy$ ,  $dz$  of 3, 3, and 1 m, respectively. Away from the injection well, the numerical mesh becomes coarse (Figure 3b). A mixed van Genuchten/Brooks Corey relative permeability<sup>33</sup> model is selected for water/CO<sub>2</sub> multiphase flow simulations and the related coefficients are adopted from references<sup>33–35</sup>. The numerical simulations start from hydrostatic conditions (gravity equilibrium) and then simulate the injection of CO<sub>2</sub> in the reservoir for 4 years. Far-field pressure on lateral and top model





**Figure 4.** Computed mean and 95% confidence intervals of the four risk proxies for 4 years.

boundaries is maintained at the initial hydrostatic pressure at all times, while the bottom boundary is fixed as no-flow. The CO<sub>2</sub> pressure at the injection point is fixed at 18.5 MPa and is based on the hydrofracture limit for the Duperow formation.<sup>19</sup> By fixing the injection pressure, we allow injection rate to vary as a function of reservoir heterogeneity and time during a 4-year simulation period (the planned duration of the Big Sky injection phase). This technique allows us to estimate the probability of the Big Sky Project reaching its goal of 1 Mt in 4 years. By the end of most realizations, the simulated CO<sub>2</sub> plume extends from 1 to 2 km in the horizontal direction (at the top of the Middle Duperow). Because supercritical CO<sub>2</sub> has a lower density than the brine in the reservoir, the injected CO<sub>2</sub> mainly migrates horizontally by pressure differences and upward by buoyancy resulting in the plume having a larger width at the upper part of the reservoir. For each realization a postprocessing step is conducted to compute statistics on three of the risk proxies, splitting the migration proxy into caprock and basement migration components including: the total CO<sub>2</sub> injection in 4 years (inj4yr), the radius of the area of review (Raor), and the migration rate into the caprock (rc) and basement (rb). Finally, the fourth risk proxy (monitoring well location) is calculated by generating a map of probability of intersecting separate phase CO<sub>2</sub> as a function of both distance and time from the start of injection.

## RESULTS AND DISCUSSION

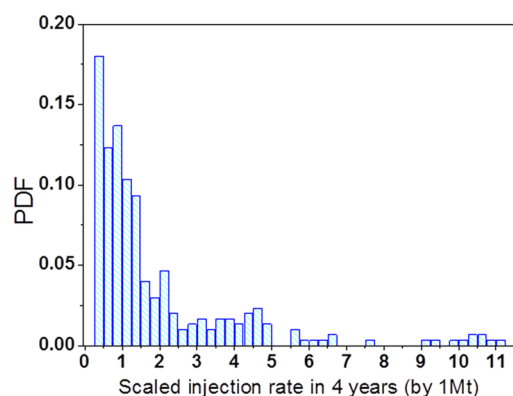
The definition of the AoR used in CO<sub>2</sub> geological sequestration is still an active topic of discussion in the sequestration community. Zhang et al.<sup>36</sup> developed a numerical method based on the vertically integrated mass per area of supercritical CO<sub>2</sub> to delineate the CO<sub>2</sub> plume extent for defining the AoR. Oldenburg and Zhou<sup>32</sup> apply EPA's AoR method<sup>37</sup> to the Big Sky project data, using the minimum elevated pressure in the injection zone that could lift brine from the injection reservoir to the deepest underground sources of drinking water. We use the results of Oldenburg and Zhou<sup>33</sup> and assume a minimum elevated pressure of 0.1 MPa to compute the radius of the AoR. Note that migration of CO<sub>2</sub> into the confining rocks reflects flow of CO<sub>2</sub> out of the Middle Duperow into the surrounding,

relatively impermeable formations. As such, this is not leakage into overlying drinking water resources but movement of CO<sub>2</sub> within the containment zone of the project (e.g., discussed by Oldenburg and Lewicki<sup>38</sup>).

**Statistics of the Risk Proxies.** By using the postprocessing results of the 300 MC simulations, we conduct a statistical analysis of the three of the risk proxies, splitting the migration proxy into caprock and basement migration components. The mean and standard deviation of the outputs are computed at 20 different time steps. By assuming that these risk proxies are normally distributed at each time step, we compute the 95% confidence intervals.<sup>39</sup> The results are shown in Figure 4. The computed mean injection in 4 years is 1.8 Mt (Figure 4a), which is larger than the 4-year injection target (1 Mt). The radius of the AoR, computed based on a reference of 0.1 MPa pressure change, has a mean, lower and upper bounds of 4.8, 3.5, and 6.3 km, respectively (Figure 4b). The mean migration amount into the caprock and basement is 0.08 and 0.012 Mt, respectively (Figure 4c and d), which means that about 5% of the injected CO<sub>2</sub> migrates into the confining rocks (e.g., caprock and basement). Note that this amount of CO<sub>2</sub> mainly remains within local higher-permeability zones of the Upper Duperow (4.4%) and Lower Duperow (0.6%) and does not migrate through the top of the capping sequence (Nisku and Potlatch formations).

For detailed analysis of the injectivity from the 300 realizations, we use the simulated injection rates at 4 years to plot a histogram of the total accumulated injection amount (Figure 5). The results indicate that about 58% of realizations have a 4-year CO<sub>2</sub> injection mass larger than 1 Mt, 70% of the realizations have a CO<sub>2</sub> injection mass larger than 0.8Mt, and 90% of the realizations have a CO<sub>2</sub> injection mass larger than 0.6 Mt. Thus, if the project is allowed to operate for an extra year, the predicted probability of a single injection well being successful stands at approximately 70%.

**Global Sensitivity Analysis.** In order to determine the key flow and transport parameters driving CO<sub>2</sub> migration behavior in the reservoir and confining rocks (basement, and caprock), global sensitivity analysis techniques were used for investigating input-output sensitivities over the entire distributions of the



**Figure 5.** Histogram of the computed CO<sub>2</sub> injection rates scaled by 1E9 kg in 4 years from 300 MC simulations. About 58% of realizations have a CO<sub>2</sub> 4-year injection rate larger than 1 Mt, 70% of the realizations have a CO<sub>2</sub> injection rate larger than 0.8 Mt, and 90% of the realizations have a CO<sub>2</sub> injection rate larger than 0.6 Mt.

uncertain parameters (Table 1). The main effect method<sup>25,40</sup> was used to quantify the impact of uncertainty and sensitivity of the input parameters. The main effect method is a variance-based analysis and it displays first-order “Sobol” indices for the response surface built from the Monte Carlo simulations.<sup>25</sup> The essence of this analysis is the statistical measure called variance of condition expectation. The variance-based analysis uses the following equation:

$$\text{VCE}(X_k) = \frac{100}{s} \sum_{j=1}^s (\bar{Y}_j - \bar{Y})^2 - \frac{1}{sr^2} \sum_{j=1}^s \sum_{i=1}^r (Y_{ij} - \bar{Y}_j)^2 \quad (4)$$

where, VCE measures the variability in the conditional expected value of  $Y$  as the input parameter  $X_k$  takes on different values,  $s$  is the number of distinct values of each input parameter, and  $r$

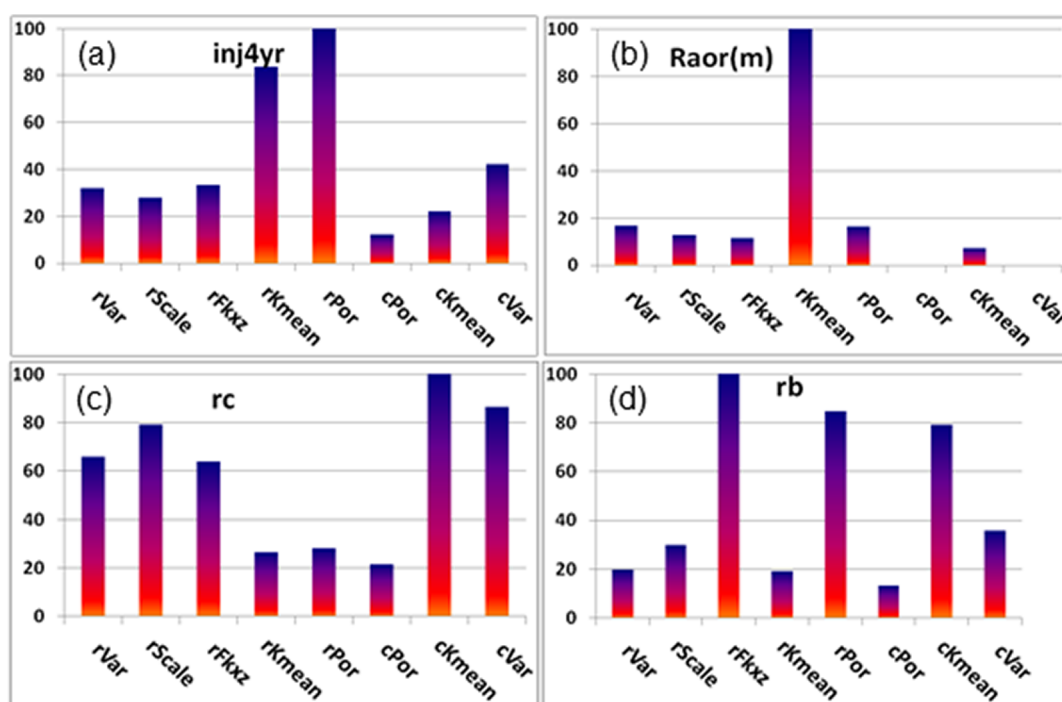
is the number of replications.  $N = sr$  is the sample size. The sensitivity of the output variable to the input parameters is quantified by eq 4 and reranked from 0 to 100 to represent the importance of the input parameters.<sup>25</sup>

By using the Monte Carlo simulation results as the input for PSUADE,<sup>25</sup> we conduct global sensitivity analysis with the main effect method for the first three risk proxies (with migration split into caprock and basement components). The results plotted in Figure 6 show that different risk proxies are sensitive to different parameters. For example, the 4-year injectivity is mainly controlled by the reservoir porosity and permeability. The radius of the AoR (which was defined by a minimum elevated pressure of 0.1 MPa in the reservoir) is most sensitive to the reservoir permeability. The CO<sub>2</sub> migration rates into the confining rocks (e.g., caprock and basement) are most sensitive to the mean permeability in these zones, as well as the permeability variance, integral scale and the anisotropy factor (Figure 6). This result indicates that the local high permeability zones in the heterogeneous confining rocks would lead to CO<sub>2</sub> migration from the storage reservoir into these zones.

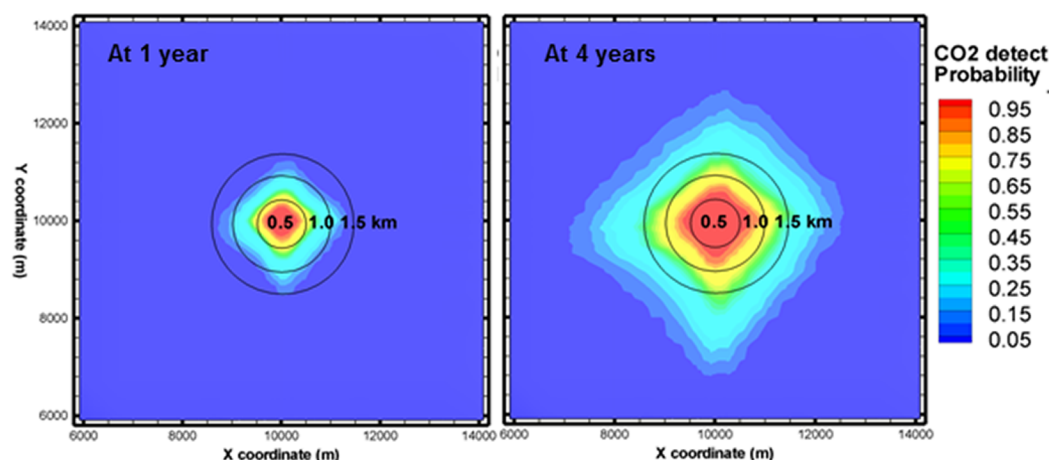
**Probability of Detecting the CO<sub>2</sub> Plume in a Monitoring Well.** By using the simulated separate phase CO<sub>2</sub> saturation data, we calculate the probability of detecting the CO<sub>2</sub> plumes at a monitoring well within the model domain using following equation:

$$P_{\text{detect}} = \frac{\sum_{i=1}^N I_i(\text{if } C_i > C_{\text{detect}})}{N} \quad (5)$$

where,  $P_{\text{detect}}$  is the probability of detection at each numerical node;  $N$  is the number of realizations (e.g., 300);  $I$  is the indicator number, which is equal to 1 if the simulated CO<sub>2</sub> saturation  $C_i$  is larger than the detection threshold  $C_{\text{detect}}$  (which is assumed to be 0.001), otherwise,  $I$  is equal to 0. The computed detection probability of the CO<sub>2</sub> plumes at 1 year and 4 years are shown in the Abstract Figure (from a cross



**Figure 6.** Global sensitivity of the four risk proxies to the eight input parameters.



**Figure 7.** CO<sub>2</sub> detect probability at the top of the reservoir (Middle Duperow) at 1 year (left) and 4 years (right).

section through the injection well) and Figure 7 (from an XY plane view at the top of the Middle Duperow). An XZ plane view of the detection probability is shown in the TOC Art Figure. After one year of injection, the predicted CO<sub>2</sub> plumes are small, and only if the monitoring well is located within 0.5 km of the injector will the CO<sub>2</sub> plumes be detected with a probability greater than 75%. After 4 years of injection, CO<sub>2</sub> plumes become much larger and monitoring wells located within 1 to 1.2 km of the injector have greater than a 75% chance of detecting CO<sub>2</sub>. Installation within 0.5 km would increase the likelihood to nearly 100% of detecting CO<sub>2</sub> by the end of the 4-year test.

**Implications.** The Integrated Monte Carlo (MC) simulations created under a probability framework constructed using regional data have allowed us to assess CO<sub>2</sub> injectivity, the area of review (AOR), migration rate into confining rocks, and the probability of detecting the injected CO<sub>2</sub> plume in monitoring wells as a function of distance from a hypothetical injection location. Global sensitivity results indicate that reservoir porosity and permeability are the key parameters controlling the CO<sub>2</sub> injectivity and the radius of the AoR. CO<sub>2</sub> migration into the confining rocks is controlled by their permeability, porosity heterogeneity, and anisotropy factor. Injectivity analysis indicates that the project goal of injecting 1 Mt in 4 years is likely despite significant uncertainty in the permeability and porosity heterogeneity. Injectivity is crucial to project success, and the finite probability of needing more than one injection well highlights the need to target data collection that will increase the likelihood of locating higher permeability/porosity volumes in the injection horizon. The calculated AoR gives an initial estimate of how many older wells located near the injection site may require remediation attention and provides planning guidance on locating far-field monitoring equipment to verify pressure changes predicted during preinjection modeling. The potential for small patches of relatively low permeability in the upper and lower Duperow suggests that a significant portion (5%) of the injected CO<sub>2</sub> could be trapped in these typically tight formations, which is a form of permanent sequestration.<sup>41</sup> The possibility that some migration may occur into these units gives the project guidance on selecting storage reservoir bounding units that are highly likely to contain the entire injected plume. This is quite important for project success because the bounding units of a geologic storage facility must be well-defined to pass review by the EPA, and definition of these boundaries is currently

flexible.<sup>42</sup> The pre-site characterization risk analysis also provides valuable guidance on locating monitoring wells, which should be within 0.5 km for a high likelihood of observing the CO<sub>2</sub> plume during the first year of injection. The goal of locating characterization wells that can later be reworked into monitoring wells has the potential to save projects significant drilling costs. The statistical methodology developed in this study can be applied to other CO<sub>2</sub> geological sequestration sites for pre-site characterization risk analysis. Risk analysis for geological carbon sequestration is an iterative process. When more site-specific reservoir parameters are obtained from drilling and injection, we will revisit the calculations of uncertain parameters to refine our estimates of risk and performance.

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### Notes

The authors declare no competing financial interest.

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